Time Accurate Simulation of Nonequilibrium Flow inside the NASA Ames Electric Arc Shock Tube

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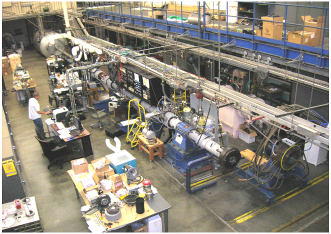
SciTech 2019 - TP-04: Non-Equilibrium Flows I

Outline

Computers vs. wind tunnels

Pleiades petascale supercomputer
NASA Advanced Supercomputing (NAS) Division



NASA Ames' Electric Arc Shock Tube*

*Successes and Challenges in Ground Testing and Simulation of Radiation and Shock Tubes.
Brett A. Cruden, AIAA AVIATION Meeting, June, 2017

In 1975, Dean R. Chapman et al. wrote about computers beginning to supplant wind tunnels within the next decade. Computers vs. wind tunnels for aerodynamic flow simulations. 1975. **Astronautics and Aeronautics, vol. 13, Apr. 1975, p. 22-30, 35.**

Dean R. Chapman

Challenges in EAST simulation

Modeling the entire facility from the arc-driver to the test section involves a large number of different physical processes !

- The arc-heating process in the driver gas requires an accurate description of the current distribution, $\rightarrow$ MHD equations need to be solved.
- The diaphragm rupture would require an understanding of the material deformation up to the plasticity limit and then rupture propagation with some degree of non-uniformity.
- Diaphragm fragments, residual soot from previous experiments and wall ablation due to high wall temperatures may contaminate the flow.
- The hot jet of the driver gas penetrating into the cold driven tube is a three-dimensional problem and involves turbulent multi-scale mixing.
- Radiative losses may need to be to be considered for certain conditions, which would require coupling the CFD code with a radiation solver.

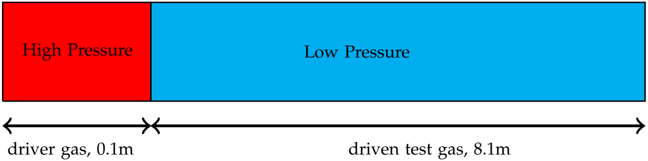
$\Longrightarrow$ The modeling of the EAST facility is a multi-scale problem and a CFD tool that accounts for all the physics, to our knowledge, does not yet exist

Assumptions

- The arc-heating process of the driver gas is not taken into account
  $\rightarrow$ The thermochemical state of the driver gas is considered in chemical and thermal equilibrium, at rest, and at a well defined constant temperature and pressure when the diaphragm breaks.
- The diaphragm is considered ideal and thus providing a simple plane discontinuity between the driver and the driven gases during the first time step.
- The boundary layer is considered as laminar.
- Radiation cooling is not accounted for during the unsteady simulation.

WHAT IS THE PROBLEM NOW ?

The "not so easy" EAST problem



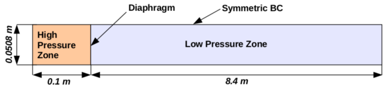
Flow in a tube with a high speed shock wave

- Modeling the complete facility requires gridding a physical length of approximately eight meters.
- Crucial flow features such as shock and contact discontinuities (CD) need to be captured and resolved with good accuracy. $\rightarrow \Delta x \approx 10^{-5}$ - 10^{-6} m.
- To resolve the boundary layers (BL) would require a grid spacing on the order $\Delta y \approx 10^{-6}$ - 10^{-7} m.
- The stiffness is increased by the chemical and kinetics source terms governing the non-equilibrium processes.

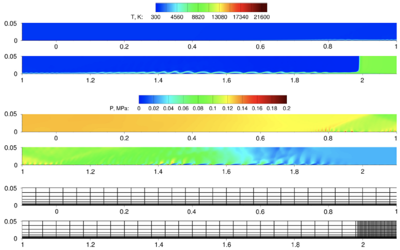
Previous work

Kotov et al. -JCP 269 (2014) 215-233)-

- Full length of the shock tube, 8 [m]
- Thermal equilibrium
- Higher-order WENO/Strang-splitting
- A grid stretching is also applied to smooth the transition from the coarse to the fine grid zone.



- Full length of the shock tube, 8 [m]



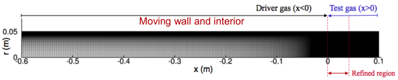
Kotov et al. JCP 269 (2014) 215-233

- Observed a Tollmien-Schlichting-like instability complex pattern near the wall.

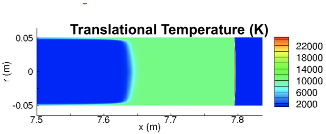
Previous work

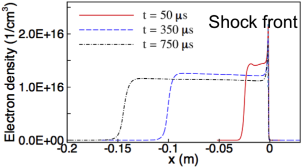
Chandel et al. (AIAA 2017-0744, AIAA 2018-1722)

- Moving frame with a constant speed close to shock-speed
- Thermo-chemical non-equilibrium
- Finite Volume, 2^{nd} order in space and 1^{st} order time implicit
- A grid stretching is applied to smooth the transition from the coarse to the fine grid zone.



- The grid covers 0.7 [m] and highly resolved near the shock





Durgesh

- The method enables a drastic reduction of the computational cost by several orders of magnitude while maintaining a high resolution of the shock and the contact

Physics and Numerics

Physical models and Numerical methods

- Full length of the shock tube, 8 [m]
- Thermal and chemical equilibrium - Park's two-temperature model
- Chapman-Enskog method for the transport properties.
- The mass diffusion fuxes are obtained by solving the Stefan-Maxwell equations under the mass conservation constraint.

$\rightarrow$ The thermodynamics and transport properties are computed using PLATO library [UIUC]

Numerical methods

$$\partial_t(r^\epsilon \mathbf{Q}) + \sum_{i\in\mathcal{D}}(r^\epsilon \partial_i \mathbf{F}_i^c) + \sum_{i\in\mathcal{D}}(r^\epsilon \partial_i \mathbf{F}_i^d) = r^\epsilon \mathbf{S}$$

$\epsilon = 1$ for axisymmetric flows and $\epsilon = 0$ for 2D ones.

- Second order Finite Volume solver
- Linearly reconstruction using a least-squares method
- The convective fluxes are computed using the $AUSM^{+UP}$ scheme.
- Crank-Nicolson scheme for time integration

Iterative solution for non-linear equations

$$\begin{cases} \mathcal{J}\left(\mathbf{s}^k\right)\Delta\mathbf{s}^k & = & -\mathcal{R}^*(\mathbf{s}^k) \\ \mathbf{s}^{k+1} & = & \mathbf{s}^k + \Delta\mathbf{s}^k \end{cases}$$

Newton iterative process
1 : Set $\mathbf{s}^{[0]} = \mathbf{u_{pred}}$
2 : for (k= 0,1,...until convergence) do
3 : Solve $\mathcal{J}(\mathbf{s}^{[k]})\Delta\mathbf{s}^{[k]} = -\mathcal{R}^*(\mathbf{s}^{[k]})$
4 : Set $\mathbf{s}^{[k+1]} = \mathbf{s}^{[k]} + \Delta\mathbf{s}^{[k]}$
5 : end for
6 : Update $\mathbf{u}^{n+1} = \mathbf{s}^{[k+1]}$

- Generalized Minimum RESidual (GMRES) algorithm and Additive Schwartz pre-conditioner - PETSc library-

CFD Solver

COOLFluiD platform

$$\partial_t Q + \nabla \cdot F^c = \nabla \cdot F^d + S$$

Multiple 1D/2D/3D parallel solvers for unstructured grids

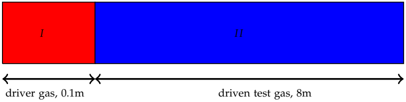
- Time Steppers : RK-n, 1- & 3-point Backward Euler, CN
- **Multiple Space Discretizations** : FV, FE, RD, DG, Spectral FV/FD
- **Multiple Linear System Solvers** : PETSc, Trilinos, Pardiso, SAMG

Multiple physical models

- Steady/unsteady **compressible and incompressible flows**
- Reactive flows : LTE, thermo-chemical nonequilibrium, ICP
- Magnetohydrodynamics (MHD), Maxwell, aeroacoustics, RANS, GReKO, LES
- Heat transfer, structural analysis, electro-chemistry

Numerical setup

- A two-dimensional uniform grid was used for this simulation - $\Delta x = 10^{-3} m$, $d_{wall} = 10^{-6}$.
- The wall is considered as isothermal at $T_w = 300K$ and no slip wall boundary conditions is applied.
- A symmetry condition was applied on the boundary with $y = 0$,
- A supersonic boundary condition is applied at the end of the driven tube.
- Wall condition is used at the end of the driver tube.
- Air -11 species - is used as a test gas, with the driver gas is composed of 99% of Helium and 1% Nitrogen.

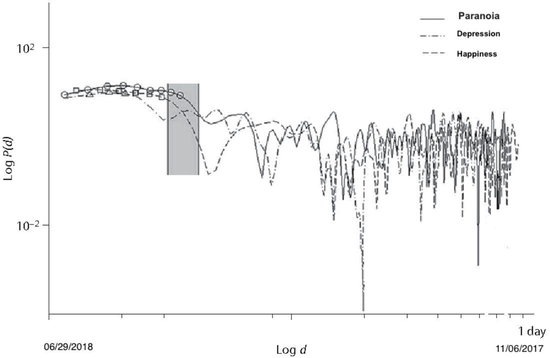


	driver	driven
	Y_{N_2} : 0.01	Y_{N_2} : 0.79
	Y_{He} : 0.99	Y_{O_2} : 0.21
ρ, kg/m^3	1.10546	3.0964 x 10^{-4}
T, K	6000	300
p, Pa	12.7116 x 10^6	26.771

TABLE – Initial conditions at diaphragm rupture

Results : Computational resources

- 500 Ivy-Bridge nodes -1000 cores-, on Pleiadaes, NASA Advanced Supercomputing (NAS)
- 120 days of continuous run and 7 months of monitoring the simulation
- 12 TB data



Impact of very long single CFD run on human body

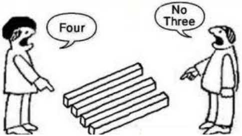
Results : flow field

Results : flow field $\nabla P(t)$

Results : centerline temperatures, $T(t) - T_v(t)$

Results : what is going on ?

- Physics ?
- Numerics ?
- Who's to blame ?

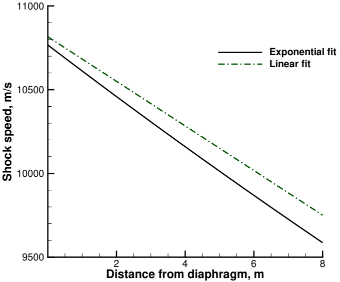


Results : flow field 2D- inviscid $\nabla P(t)$

Results : flow field 2D- axisymmetric inviscid $\nabla P(t)$

Results : shock speed

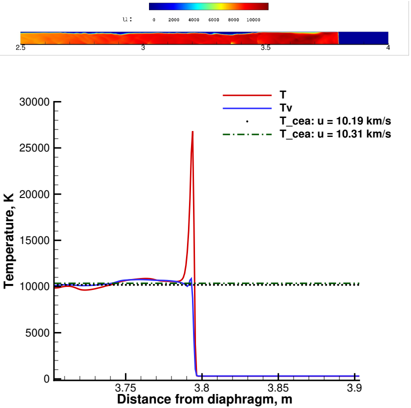
- The shock speed has been calculated based on 10% pressure rise with respect test gas initial fill pressure.
- Two fit strategies were applied using an exponential and a linear method.

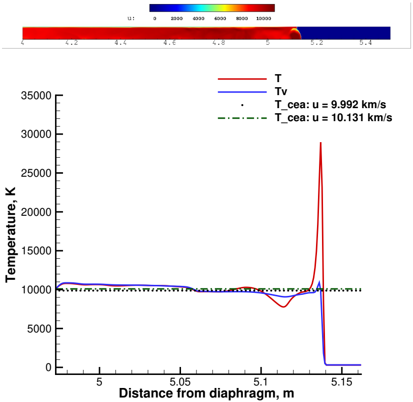


Position, m	3.79	5.14	6.26	7.76
Shock Speed -exp fit-, m/s	10189	9992	9831	9619
$T^{cea}_{equilibiurm}$, K	10180	9875	9599	9188
Shock Speed -lin fit-, m/s	10310	10131	9982	9782
$T^{cea}_{equilibiurm}$, K	10352	10093	9859	9509

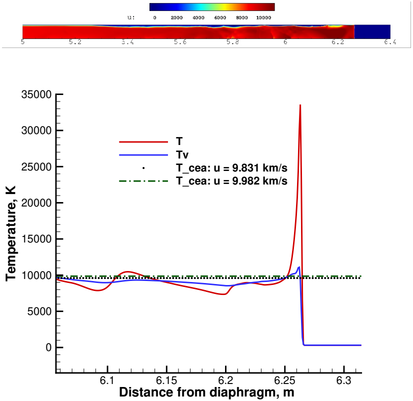
TABLE – Shock speed at different locations

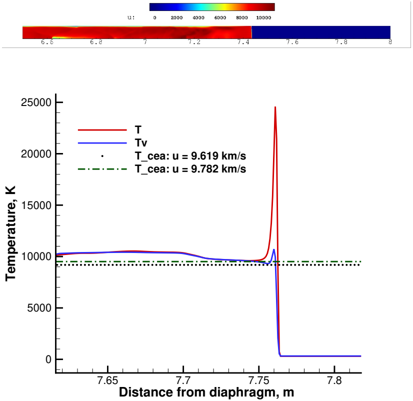
Results


u:
0
2000
4000
6000
8000
10000
2.5
3
3.5
4
T
Tv
T_cea: u = 10.19 km/s
T_cea: u = 10.31 km/s
Temperature, K
0
5000
10000
15000
20000
25000
30000
3.75
3.8
3.85
3.9
Distance from diaphragm, m


u:
0
2000
4000
6000
8000
10000
4
4.2
4.4
4.6
4.8
5
5.2
5.4
T
Tv
T_cea: u = 9.992 km/s
T_cea: u = 10.131 km/s
Temperature, K
0
5000
10000
15000
20000
25000
30000
35000
5
5.05
5.1
5.15
Distance from diaphragm, m

Results


u:
0
2000
4000
6000
8000
10000
5
5.2
5.4
5.6
5.8
6
6.2
6.4
Temperature, K
35000
30000
25000
20000
15000
10000
5000
0
T
Tv
T_cea: u = 9.831 km/s
T_cea: u = 9.982 km/s
6.1
6.15
6.2
6.25
6.3
Distance from diaphragm, m


u:
0
2000
4000
6000
8000
10000
6.6
6.8
7
7.2
7.4
7.6
7.8
8
Temperature, K
25000
20000
15000
10000
5000
0
T
Tv
T_cea: u = 9.619 km/s
T_cea: u = 9.782 km/s
7.65
7.7
7.75
7.8
Distance from diaphragm, m

Conclusion

- A time accurate simulation of the thermo-chemical non-equilibrium flow inside the EAST facility was performed using a two-dimensional second-order axisymmetric finite volume solver.
- It was found that the axisymmetric source term generates a numerical instability that appears as shock bending. This instability is time dependent which greatly affects the shock speed.
- Translational and vibrational temperatures profiles were compared to CEA equilibrium prediction. Good agreement was obtained with CEA prediction close to the test-section (shock location is at 7.6 m from the diaphragm) and just behind the shock
- Full equilibrium is not achieved due to the deceleration of the shock and the effect of shock bending.

Future work

- Three-dimensional (axisymmetric) simulation will be performed, which we believe will alleviate the instability problem of the axisymmetric source term
- Current axial grid resolution is not sufficient to capture the correct waves speeds, an optimal grid would have a higher resolution only in the region of interest i.e 20 cm behind the shock, thus r-adaptation will be explored.

Acknowledgments

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- Tim Sandstrom at the NASA Advanced Supercomputing (NAS) visualization team
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